4-Propionyl-4'-n-octanoyloxyazobenzene

Inchi: InChI=1S/C23H28N2O3/c1-3-5-6-7-8-9-23(27)28-21-16-14-20(15-17-21)25-24-19-12-10-
InchiKey: FTZUNRYKMRDWTB-OCOZRVBESA-N
Formula: C23H28N2O3
SMILES: CCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CC)cc2)cc1
Mol. weight [g/mol]: 380.48
CAS: 76204-64-3

Physical Properties

Property code	Value	Unit	Source
hf	-378.09	kJ/mol	Joback Method
hvap	95.24	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.961		Crippen Method
mcvol	312.080	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
tb	1068.32	K	Joback Method
tc	1312.86	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.49	kJ/mol	369.65	NIST Webbook
sfust	74.36	J/mol×K	369.65	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76204643&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature